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NEWS 15 FEB 11
                 WTEXTILES reloaded and enhanced
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=> d 13 1-7 ibib ab hitstr

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:281174 CAPLUS

DOCUMENT NUMBER: 146:330828

TITLE: Pharmaceutical compositions containing  $\alpha-4$  integrin mediated cell adhesion inhibitors

INVENTOR(S): Ward, Robert William; Witherington, Jason

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 38pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
JP 2007063268 PRIORITY APPLN. INFO.:	A	20070315	JP 2006-212923 JP 2005-227980 A	20060804 20050805		
OTHER SOURCE(S):	MARPAT	146:330828	01 2000 22,300	2000000		

AB The invention relates to a pharmaceutical composition characterized by containing a

compound I [A, B, D = aryl, heteroaryl; R1, R2, R3 = C1-6 alkyl, halogen, C1-6 alkoxy, hydroxy, cyano, CF3, OCF3, nitro, C1-6 alkylthio, amino, mono-(di-)-C1-6 alkylamino, carboxy, C1-6 alkanoyl, amido, mono-(di-)-C1-6 alkylamido, etc; R4, R4' = H, C1-6 alkyl, halogen, C1-6 alkoxy; V = O, S, NH, N-C1-6 alkyl, NNO2, NCN; W, X, Y, Z = C, CH, N, wherein at least on of X, Y, and Z is N; L = -(CH2)q-, -(CH2)q'O-, wherein q = 0=3, q' = 2, 3; J = -CR5:CR6-, wherein R5, R6 = H, C1-6 alkyl, single bond, etc.; m, n, p = 0-3; t = 0-2], or its pharmaceutically acceptable derivative as an active component. The compound has an inhibitory effect against  $\alpha$ -4 integrin mediated cell adhesion, and is suitable for use for treatment of  $\alpha$ -4 integrin mediated cell adhesion-related disease, e.g. asthma, enteritis, rheumatic arthritis, and multiple sclerosis, etc. For example, a compound (R,S)-3-[4-[5-[3-ethoxy-4-(3-o-tolylureido)phenyl]-6-oxo-6H-pyrimidin-1-ylmethyl]phenyl]butyric acid was prepared, and examined for its interaction with integrin VLA-4 in vitro.

IT 862855-36-5P 862855-37-6P 862855-38-7P 862855-39-8P 862855-42-3P 862855-43-4P 862855-44-5P 862855-45-6P 862855-47-8P 862855-48-9P 862855-49-0P 862855-50-3P 862855-51-4P 862855-52-5P 862855-53-6P 862855-54-7P 928080-46-0P 928080-53-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pharmaceutical compns. containing  $\alpha\!-\!4$  integrin mediated cell adhesion inhibitors)

RN 862855-36-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyrazinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-37-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyrazinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

RN 862855-38-7 CAPLUS

CN Benzenepropanoic acid, 4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- (CA INDEX NAME)

RN 862855-39-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-42-3 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

RN 862855-43-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-,  $(\beta S)$ - (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-44-5 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-ethoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl- (CA INDEX NAME)

RN 862855-45-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

RN 862855-47-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-48-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-49-0 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyrazinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

RN 862855-50-3 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- $\beta-methyl- (CA INDEX NAME)$ 

RN 862855-51-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-52-5 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math display="inline">\beta-methyl-$ , ( $\beta$ S)- (CA INDEX NAME)

RN 862855-53-6 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2, <math>4-dimethyl-6-oxo-1(6H)-pyrimidinyl]methyl]-\beta-methyl-$ , ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-54-7 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, sodium salt (1:1), ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Na

RN 928080-46-0 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-

, sodium salt (1:1),  $(\beta R)$  - (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{HO}_2\text{C} \\ \text{R} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{Me} \\ \text{O} \end{array}$$

Na

RN 928080-53-9 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, sodium salt (1:1), ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

Na

IT 862855-64-9P 862855-78-5P 862855-91-2P

862855-96-7P 928082-53-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pharmaceutical compns. containing  $\alpha\text{--}4$  integrin mediated cell adhesion inhibitors)

RN 862855-64-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-ethoxy-4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- $\beta-methyl-$, ethyl ester (CA INDEX NAME)$ 

RN 862855-78-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-91-2 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-96-7 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2, <math>4-dimethyl-6-oxo-1(6H)-pyrimidinyl]methyl]-\beta-methyl-$ , methyl ester, ( $\beta R$ )- (CA INDEX NAME)

RN 928082-53-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:1001119 CAPLUS

DOCUMENT NUMBER: 146:213

TITLE: Pyridone derivatives as potent, orally bioavailable

VLA-4 integrin antagonists

AUTHOR(S): Witherington, Jason; Blaney, Emma L.; Bordas, Vincent;

Elliott, Richard L.; Gaiba, Alessandra; Garton, Neil; Green, Philip M.; Naylor, Antoinette; Smith, David G.; Spalding, David J.; Takle, Andrew K.; Ward, Robert W.

CORPORATE SOURCE: Department of DMPK and Medicinal Chemistry, Neurology

and GI Centre of Excellence for Drug Discovery,

GlaxoSmithKline Research Limited, Essex, CM19 5AW, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(21), 5538-5541

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:213

AB A series of pyridone-N-benzylpropanoic acids have been optimized to afford potent orally bioavailable VLA-4 antagonists.

IT 915157-69-6 915157-73-2 915157-74-3

915157-75-4 915157-76-5

RL: PAC (Pharmacological activity); BIOL (Biological study) (optimization of pyridone-N-benzylpropanoic acids as orally bioavailable VLA-4 integrin antagonists)

RN 915157-69-6 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[3-methoxy-4-[[[[2-(1-methylethyl)phenyl]amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 915157-73-2 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2,3-dimethylphenyl)amino]carbonyl]amino]-3-methoxyphenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 915157-74-3 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2,4-dimethylphenyl)amino]carbonyl]amino]-3-methoxyphenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 915157-75-4 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2,5-dimethylphenyl)amino]carbonyl]amino]-3-methoxyphenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 915157-76-5 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2,6-dimethylphenyl)amino]carbonyl]amino]-3-methoxyphenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

IT 660439-96-3

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); BIOL (Biological study)

(optimization of pyridone-N-benzylpropanoic acids as orally bioavailable VLA-4 integrin antagonists)

RN 660439-96-3 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 660439-93-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-

methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl](CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-NH-C-NH$ 

RN 660440-22-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 660440-23-3 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C} \\ \text{R} \\ \text{O} \\ \text{N} \\ \text{H} \\ \text{O} \\ \text{Me} \\ \text{O} \\ \end{array}$$

RN 915157-77-6 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-,  $(\beta S)$ - (CA INDEX NAME)

RN 915157-78-7 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-79-8 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-chloro-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- $\beta-methyl-, ($\beta R)- (CA INDEX NAME)$ 

Absolute stereochemistry.

RN 915157-80-1 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]-3-(trifluoromethoxy)phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-81-2 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-ethoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-82-3 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-ethyl-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-83-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[3-methyl-4-[[(2-

methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-84-5 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[2-chloro-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-85-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[2-methyl-4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-86-7 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[3-chloro-4-[[[(2-

methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- $\beta$ -methyl-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-87-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]-3-(trifluoromethoxy)phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-88-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-ethoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ S)- (CA INDEX NAME)

RN 915157-89-0 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-ethyl-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-90-3 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[3-methyl-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 915157-91-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[2-chloro-4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ S)- (CA INDEX NAME)

RN 915157-93-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[2-methyl-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

IT 926010-03-9P

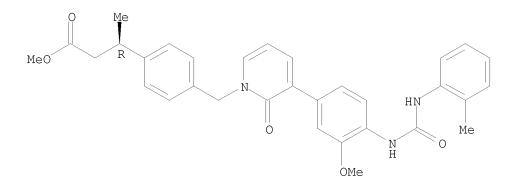
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(optimization of pyridone-N-benzylpropanoic acids as orally bioavailable VLA-4 integrin antagonists)

RN 926010-03-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- <math>\beta$ -methyl-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:453930 CAPLUS

DOCUMENT NUMBER: 144:480470

TITLE: Pyridone derivatives as potent and selective VLA-4

integrin antagonists. [Erratum to document cited in

CA144:403837]

AUTHOR(S): Witherington, Jason; Bordas, Vincent; Gaiba,

Alessandra; Green, Phil M.; Naylor, Antoinette; Parr, Nigel; Smith, David G.; Takle, Andrew K.; Ward, Robert

W.

CORPORATE SOURCE: Department of Medicinal Chemistry, Neurology & GI

Centre of Excellence for Drug Discovery,

GlaxoSmithKline Research Limited Harlow, Essex, CM19

5AW, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(12), 3341

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

AB The legends to Figures 1b and 3b are incorrect. In Figure 1b, the legend should read: "GASP molecular overlay of 8 (green) and 5 (yellow)". In Figure 3b, the legend should read: "Molecular overlay of 8 (green) and 10 (yellow)".

IT 660439-93-0P 660439-96-3P 660439-99-6P

884348-00-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pyridone derivs. as potent and selective VLA-4 integrin antagonists (Erratum))

RN 660439-93-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-NH-C-NH$ 

RN 660439-96-3 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-NH-C-NH$ 

RN 660439-99-6 CAPLUS

CN Benzoic acid, 4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 884348-00-9 CAPLUS

CN Benzeneacetic acid, 4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

IT 660440-04-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(pyridone derivs. as potent and selective VLA-4 integrin antagonists (Erratum))

RN 660440-04-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester (CA INDEX NAME)

L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:232883 CAPLUS

DOCUMENT NUMBER: 144:403837

TITLE: Pyridone derivatives as potent and selective VLA-4

integrin antagonists

AUTHOR(S): Witherington, Jason; Bordas, Vincent; Gaiba,

Alessandra; Green, Phil M.; Naylor, Antoinette; Parr, Nigel; Smith, David G.; Takle, Andrew K.; Ward, Robert

W.

CORPORATE SOURCE: Department of Medicinal Chemistry, Neurology & GI

Centre of Excellence for Drug Discovery,

GlaxoSmithKline Research Limited, Essex, CM19 5AW, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(8), 2256-2259

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:403837

AB A novel series of pyridone inhibitors has been identified through pharmacophore anal., as potent antagonists of VLA-4. Analog I exhibited excellent inhibitory potency.

IT 660439-93-0P 660439-96-3P 660439-99-6P

884348-00-9P

RN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pyridone derivs. as potent and selective VLA-4 integrin antagonists)  $660\,439-93-0$  CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-NH-C-NH$ 

RN 660439-96-3 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-NH-C-NH$ 

RN 660439-99-6 CAPLUS

CN Benzoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{HO}_2\text{C} \\ \text{CH}_2 \\ \text{O} \\ \end{array}$$

RN 884348-00-9 CAPLUS

CN Benzeneacetic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

$$HO_2C-CH_2$$
 $CH_2-N$ 
 $NH-C-NH$ 

IT 660440-04-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(pyridone derivs. as potent and selective VLA-4 integrin antagonists)

RN 660440-04-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-

methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-,
methyl ester (CA INDEX NAME)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1025806 CAPLUS

DOCUMENT NUMBER: 143:299147

TITLE: Medicine compositions containing pyridone analogs for

inhibiting  $\alpha 4$ -integrin-mediated cell adhesion Witherington, Jason; Elliott, Richard Leonard

INVENTOR(S): Witherington, Jason; Elliott, Ric PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 36 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE		DATE	
				_	
JP 2005255675	A	20050922	JP 2005-33237		20050209
PRIORITY APPLN. INFO.:			JP 2004-31901	Α	20040209
		4 40 0004 45			

OTHER SOURCE(S): MARPAT 143:299147

AB Medicine compns. containing pyridone analogs and their pharmacol. acceptable salts are claimed for inhibiting  $\alpha 4$ -integrin-mediated cell adhesion for treatment of related diseases, including chronic inflammatory

diseases, asthma, allergy, inflammatory bowel disease, rheumatoid arthritis, atopic dermatitis, multiple sclerosis, organ transplant rejection, cardiovascular disease, diabetes, tumor, central nervous system diseases, etc.

G1Seases, etc.

IT 660439-93-0P 660439-96-3P 660439-98-5P 660439-99-6P 660440-00-6P 660440-03-9P 660440-04-0P 660440-06-2P 660440-08-4P 660440-09-5P 660440-10-8P 660440-11-9P 660440-14-2P 660440-20-0P 660440-21-1P 660440-22-2P 660440-23-3P 660440-24-4P 660440-25-5P 660440-26-6P 660440-27-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(medicine compns. containing pyridone analogs for inhibiting  $\alpha 4\text{--integrin-mediated}$  cell adhesion and treating related diseases) 660439--93--0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

RN 660439-96-3 CAPLUS

RN

CN Benzenepropanoic acid, 4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 660439-98-5 CAPLUS

CN Benzenepropanoic acid, 4-[[5-chloro-3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

RN 660439-99-6 CAPLUS

CN Benzoic acid, 4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 660440-00-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH} \\ \text{CH}_2-\text{NH}-\text{C}-\text{NH} \\ \end{array}$$

RN 660440-03-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- $\beta-methyl- (CA INDEX NAME)$ 

RN 660440-04-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester (CA INDEX NAME)

RN 660440-06-2 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ethyl ester (CA INDEX NAME)

RN 660440-08-4 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, [[(cyclohexyloxy)carbonyl]oxy]methyl ester (CA INDEX NAME)

PAGE 1-B

RN 660440-09-5 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, [[(1-methylethoxy)carbonyl]oxy]methyl ester (CA INDEX NAME)

PAGE 1-B

RN 660440-10-8 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

PAGE 1-B



RN 660440-11-9 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, 1-methylethyl ester (CA INDEX NAME)

RN 660440-14-2 CAPLUS

CN Phenylalanine, N-acetyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 660440-20-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(3-fluoro-2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-N$ 
 $NH-C-NH$ 
 $Me$ 

RN 660440-21-1 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[2-fluoro-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

RN 660440-22-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 660440-23-3 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 660440-24-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- $\beta-phenyl- (CA INDEX NAME)$ 

$$\begin{array}{c} \text{Ph} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH} \\ \text{CH}_2-\text{NH}-\text{C}-\text{NH} \\ \end{array}$$

RN 660440-25-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 660440-26-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 660440-27-7 CAPLUS

CN Benzenepropanoic acid,  $\beta$ ,  $\beta$ -dimethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

IT 660440-58-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(medicine compns. containing pyridone analogs for inhibiting  $\alpha 4\text{-integrin-mediated}$  cell adhesion and treating related diseases)

RN 660440-58-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester (CA INDEX NAME)

ANSWER 6 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:823674 CAPLUS

DOCUMENT NUMBER: 143:229873

TITLE: Preparation of 2-(phenylmethyl)pyrimidinones and

related compounds as alpha-4 integrin mediated cell adhesion inhibitors for the treatment of inflammatory

diseases

INVENTOR(S): Ward, Robert William; Witherington, Jason

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.					KIND DATE												
	WO 2005075438			A1 20050818			WO 2005-JP2194											
		W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
			NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
			ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
		RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
			EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,
			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,
			MR,	ΝE,	SN,	TD,	ΤG											
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	ΕP	1737	826			A1		2007	0103		EP 2	005-	7101	95		2	0050.	208
		R:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	IE,
			IS,	ΙT,	LI,	LT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR		
	CN 1918133				A 20070221								20050208					
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	US	2008	0234	301		A1		2008	0925		US 2	006-	5882	35		2	0060	803
PRIOF	RITS	APP:	LN.	INFO	.:						GB 2	004-	2812		i	A 2	0040	209
											WO 2		_			W 2	0050.	208
OTHER	S	DURCE	(S):			CASI	REAC	T 14	3:229	9873	; MA	RPAT	143	:2298	373			
AB	Tit	tle c	ompd	s. I	[R1	' =	(R1)	m; R	2 <b>'</b> =	(R2	)n;	D =	(CH2	)t; I	33' =	= (R	3)p;	R1,
	R2,	. R3 =	= al:	kyl,	hal	o, a.	lkox	y, e	tc.;	R4,	R4'	= H	, al	kyl,	hal	o, et	tc.;	V = 0

S, NH, etc.; W, X, Y, Z = C, CH, N, subject to the proviso that at least one X Y and Z is N; L = (CH2)q, (CH2)q'O; J = bond, CR5 = CR6, CHR7CHR8, etc.; R5, R6 = H, alkyl; R7, R8 = H, alkyl, cycloalkyl, etc.; q = 0-3; q'= 2,3; A, B, D = aryl, heteroaryl; m, n, p = 0-3; t = 0-2] and their pharmaceutically acceptable salts were prepared For example, saponification of Et

ester II (G = OEt) afforded carboxylic acid II (G = OH). Compoounds I are claimed to be useful as alpha-4 integrin mediated cell adhesion inhibitors

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(no data provided).
ΤТ
     862855-36-5P 862855-37-6P 862855-38-7P
     862855-39-8P 862855-40-1P 862855-41-2P
     862855-42-3P 862855-43-4P 862855-44-5P
     862855-45-6P 862855-46-7P 862855-47-8P
     862855-48-9P 862855-49-0P 862855-50-3P
     862855-51-4P 862855-52-5P 862855-53-6P
     862855-54-7P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of 2-(phenylmethyl)pyrimidinones and related compds. as alpha-4
        integrin mediated cell adhesion inhibitors for the treatment of
        inflammatory diseases)
RN
     862855-36-5 CAPLUS
CN
     Benzenepropanoic acid, \beta-methyl-4-[[3-[4-[[(2-
     methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyrazinyl]methyl]-,
     (\beta R) - (CA INDEX NAME)
```

Absolute stereochemistry.

RN 862855-37-6 CAPLUS CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyrazinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-38-7 CAPLUS
CN Benzenepropanoic acid, 4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl](CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-N$ 
 $NH-C-NH$ 

RN 862855-39-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C} \\ \text{R} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{Me} \\ \text{O} \\ \text{Me} \\ \text{O} \\$$

RN 862855-40-1 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ \text{HO}_2\text{C} & & & \\ \hline \\ \text{R} & & & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \\ \text{N} & \\ \hline \\ \text{N} & \\ \hline$$

RN 862855-41-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

RN 862855-42-3 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-43-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-44-5 CAPLUS

CN Benzenepropanoic acid, 4-[[5-[3-ethoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-  $\beta$ -methyl- (CA INDEX NAME)

RN 862855-45-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C} \\ & \text{R} \\ & \text{N} \\ & \text{N} \\ & \text{O} \\ & \text{H} \\ & \text{O} \\ & \text{Me} \\ \end{array}$$

RN 862855-46-7 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ \text{HO}_2\text{C} & & & \\ \hline & & & \\ \text{R} & & & \\ \hline & & & \\ \text{N} & & \\ \hline & & \\ \text{O} & & \\ \hline & & \\ \text{Me} & \\ \end{array}$$

RN 862855-47-8 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-48-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-49-0 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyrazinyl]methyl]- <math>\beta$ -methyl-,  $(\beta R)$ - (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-50-3 CAPLUS

CN Benzenepropanoic acid, 4-[[2,4-dimethyl-5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-  $\beta$ -methyl- (CA INDEX NAME)

RN 862855-51-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-52-5 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-53-6 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2,4-dimethyl-6-oxo-1(6H)-pyrimidinyl]methyl]-<math>\beta$ -methyl-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-54-7 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, sodium salt (1:1), ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Na

CN Benzenepropanoic acid,  $4-[[5-[3-ethoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, ethyl ester (CA INDEX NAME)

RN 862855-78-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyridazinyl]methyl]-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-91-2 CAPLUS

CN Benzenepropanoic acid,  $4-[[2,4-dimethyl-5-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]- <math>\beta$ -methyl-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 862855-96-7 CAPLUS

CN Benzenepropanoic acid,  $4-[[5-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2, <math>4-dimethyl-6-oxo-1(6H)-pyrimidinyl]methyl]-\beta-methyl-$ , methyl ester, ( $\beta R$ )- (CA INDEX NAME)

Absolute stereochemistry.

RN 928082-53-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[5-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-6-oxo-1(6H)-pyrimidinyl]methyl]-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:143107 CAPLUS

DOCUMENT NUMBER: 140:199207

TITLE: Preparation of pyridones as inhibitors of  $\alpha 4$ 

integrin-mediated cell adhesion.

INVENTOR(S): Witherington, Jason; Elliott, Richard Leonard

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2004014859	A2 200402		20030808
WO 2004014859	A3 200404		
W: AE, AG, AL,	AM, AT, AU, A	AZ, BA, BB, BG, BR, BY,	BZ, CA, CH, CN,
CO, CR, CU,	CZ, DE, DK, D	DM, DZ, EC, EE, ES, FI,	GB, GD, GE, GH,
GM, HR, HU,	ID, IL, IN, I	IS, JP, KE, KG, KP, KR,	KZ, LC, LK, LR,
LS, LT, LU,	LV, MA, MD, M	MG, MK, MN, MW, MX, MZ,	NI, NO, NZ, OM,
PG, PH, PL,	PT, RO, RU, S	SC, SD, SE, SG, SK, SL,	SY, TJ, TM, TN,
TR TT T7	HA. HG. HS. F	IZ. VC. VN. YII. ZA. ZM.	7.W

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                                                                    20030808
     AU 2003256069
                                20040225
                                            AU 2003-256069
                          Α1
                                                                    20030808
     EP 1539696
                          Α2
                                20050615
                                            EP 2003-784602
                                                                    20030808
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     CN 1688548
                                20051026
                                            CN 2003-823831
                                                                    20030808
                          Α
     JP 2005535702
                          Τ
                                20051124
                                            JP 2004-527373
                                                                    20030808
     US 20050288337
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                                            US 2005-524028
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                                20080812
PRIORITY APPLN. INFO.:
                                            GB 2002-18630
                                                                 Α
                                                                   20020810
                                            WO 2003-JP10119
                                                                 W
                                                                    20030808
                         MARPAT 140:199207
OTHER SOURCE(S):
     Title compds. [I; A, B = aryl, heteroaryl; Q = C, CH; QV, QD = 5-7
AΒ
     membered heterocyclyl; D = H, alkyl; R1-R3 = alkyl, halo, alkoxy, OH,
     cyano, CF3, NO2, alkylthio, amino, CO2H, alkanoyl, amido, NHCOR9, NHSO2R9;
     R9 = alkyl, cycloalkyl, (substituted) Ph etc.; R4 = H, alkyl, halo,
     alkoxy; V = O, S, amino, NNO2, NCN; W, X, Y, Z = C, CH, CH2; dotted line =
     single or double bond; L = (CH2)r, (CH2)rrO; r = 0-3; rr = 2, 3; J =
     CR5:CR6, CHR7CHR8, single bond, CHR6; OCHR10, etc.; R5, R6, R10 = H,
     alkyl; R7, R8 = H, alkyl, cycloalkyl, aryl, heteroaryl, etc.; m, n, p =
     0-3; q = 0-2], were prepared as inhibitors of \alpha 4 integrin-mediated
     cell adhesion (no data). Thus, Et
     3-[4-[2-oxo-3-[4-(3-o-tolylureido)phenyl]-2H-pyridin-1-
     ylmethyl]phenyl]propionate and LiOH were stirred at 60° for 30 min
     in THF/H2O to give after acidification with HCl
     3-[3-[2-oxo-3-[4-(3-o-tolylureido)phenyl]-2H-pyridin-1-
     ylmethyl]phenyl]propionic acid.
     660440-06-2P
ΙT
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of pyridones as inhibitors of \alpha 4 integrin-mediated cell
        adhesion)
RN
     660440-06-2 CAPLUS
CN
     Benzenepropanoic acid, 4-[[3-[4-[[(2-
     methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-,
     ethyl ester (CA INDEX NAME)
```

$$\begin{array}{c} O \\ \\ EtO-C-CH_2-CH_2 \\ \\ CH_2-N \\ \\ O \end{array} \\ \begin{array}{c} Me \\ \\ NH-C-NH \\ \\ \end{array}$$

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IT 660439-93-0P 660439-96-3P 660439-98-5P 660439-99-6P 660440-00-6P 660440-03-9P 660440-04-0P 660440-08-4P 660440-09-5P 660440-10-8P 660440-11-9P 660440-14-2P 660440-20-0P 660440-21-1P 660440-22-2P 660440-23-3P 660440-24-4P 660440-25-5P 660440-26-6P 660440-27-7P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridones as inhibitors of  $\alpha 4$  integrin-mediated cell adhesion)

RN 660439-93-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $CH_2-N$ 
 $NH-C-NH$ 

RN 660439-96-3 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

RN 660439-98-5 CAPLUS

CN Benzenepropanoic acid, 4-[[5-chloro-3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

RN 660439-99-6 CAPLUS

CN Benzoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 660440-00-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH} \\ \\ \text{CH}_2-\text{NH}-\text{C}-\text{NH} \\ \\ \end{array}$$

RN 660440-03-9 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- $\beta-methyl-$ (CA INDEX NAME)$ 

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH} \\ \\ \text{CH}_2-\text{NH} \\ \\ \text{O} \\ \end{array}$$

RN 660440-04-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ MeO-C-CH_2-CH_2 & O & Me \\ \hline \\ CH_2-NH-C-NH & O & \\ \end{array}$$

RN 660440-08-4 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-,

[[(cyclohexyloxy)carbonyl]oxy]methyl ester (CA INDEX NAME)

PAGE 1-B

RN 660440-09-5 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, [[(1-methylethoxy)carbonyl]oxy]methyl ester (CA INDEX NAME)

PAGE 1-B

RN 660440-10-8 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

PAGE 1-B

RN 660440-11-9 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, 1-methylethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ \hline i-PrO-C-CH_2-CH_2 & MH-C-NH \\ \hline \end{array}$$

RN 660440-14-2 CAPLUS

CN Phenylalanine, N-acetyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

RN 660440-20-0 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[4-[[[(3-fluoro-2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-(CA INDEX NAME)

RN 660440-21-1 CAPLUS

CN Benzenepropanoic acid, 4-[[3-[2-fluoro-4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 660440-22-2 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 660440-23-3 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 660440-24-4 CAPLUS

CN Benzenepropanoic acid,  $4-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- $\beta-phenyl- (CA INDEX NAME)$ 

$$\begin{array}{c|c} Ph & & & \\ HO_2C-CH_2-CH & & & \\ & & & \\ & & & \\ CH_2-N & & \\ & & & \\ \end{array}$$

RN 660440-25-5 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 660440-26-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -ethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 660440-27-7 CAPLUS

CN Benzenepropanoic acid,  $\beta$ ,  $\beta$ -dimethyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{C} \\ \text{Me} \\ \text{CH}_2-\text{N} \\ \text{O} \\ \end{array}$$

IT 660440-58-4

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of pyridones as inhibitors of  $\alpha 4$  integrin-mediated cell adhesion)

RN 660440-58-4 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester (CA INDEX NAME)

IT 660440-49-3P 660440-50-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyridones as inhibitors of  $\alpha 4$  integrin-mediated cell adhesion)

RN 660440-49-3 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester, ( $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 660440-50-6 CAPLUS

CN Benzenepropanoic acid,  $\beta$ -methyl-4-[[3-[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxo-1(2H)-pyridinyl]methyl]-, methyl ester, ( $\beta$ S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).